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ON THE CAPTURE OF ELECTRONS BY FAST IONS

by

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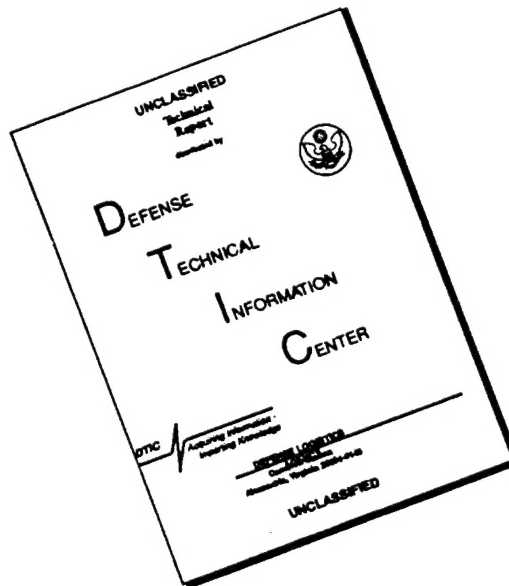
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ABSTRACT

The Oppenheimer-Brinkman-Kramers theory of the capture of electrons by alpha particles in their passage through matter is formulated in terms of a momentum representation of the electrons. For a heavy ion carrying a core of electrons, capture is largely into excited states. Total cross sections for such ions are estimated assuming hydrogen-like representations for the electron in the captured states and treating the atom from which capture takes place by the Thomas-Fermi model.

# 1. INTRODUCTION

The capture of an electron by an energetic ion in its passage through air or other material is a collision process in which an electron jumps from an atom to a bound state of the ion and the difference in energy is absorbed in the translational energy of the two heavy particles. Radiative capture can occur<sup>1</sup>, but its probability is smaller by a factor of the order of magnitude of  $(e^2/hc)^3 \approx (1/137)^3$ .

<sup>1</sup> J. R. Oppenheimer, Phys. Rev. 31, 349 (1928). J. F. Carlson has recently made detailed calculations on the radiative capture cross section (unpublished).

An estimate of the capture cross section  $\sigma_c$  has recently been made by Bohr<sup>2</sup>. His formula can be written as follows:

$$\frac{\sigma_c}{\pi a_0^2} = \frac{Z_a^{1/3}}{16i} \left( \frac{2iv_0}{v} \right)^6 \quad (1)$$

where  $a_0$  is the radius of the smallest Bohr orbit of hydrogen ( $\pi a_0^2 = 0.88 \cdot 10^{-16} \text{ cm}^2$ ),  $v_0 = e^2/h = 2.19 \cdot 10^8 \text{ cm/sec}$ ,  $v$  is the velocity of the ion,  $i$  its effective charge number, and  $Z_a$  is the atomic number of the substance through which the ion is passing. The formula is to apply for ion velocities for which

<sup>2</sup> N. Bohr (1948) Kgl. Dan. Vid. Sels. 18, 8 (1940).

$2iv_0/v \sim 1$ , and is for a stripped particle, ( $i = Z$ , where  $Z$  is the atomic number of the ion).

The Born approximation has been used by Oppenheimer<sup>1</sup> and by Brinkman and Kramers<sup>3</sup> to calculate the capture cross section of fast alpha particles. The approximation is valid only if  $2v_a/v \ll 1$  and  $2v_e/v \ll 1$ , where  $v_a$  and  $v_e$  are the orbital velocities of the electron in the initial (atomic) state and in the most tightly bound final (ionic) state, respectively. However, the results are of some interest for ion velocities below the limits of validity of the calculations.

For a stripped particle of high velocity, the principal contribution to the total capture cross section arises from capture into one of the lowest ( $n = 1$ ) electronic states of the ion, which states are widely separated in energy from the excited states. Capture into all excited states adds only twenty per cent to the cross section at high velocities<sup>1</sup> but is of greater relative importance at low velocities.

A particle carrying a single electron in a 1s state has a cross section for capture into the remaining 1s state which contains the statistical factor  $1/4$ , because the two electrons must form a singlet state of the ion. Since excited states are practically hydrogen-like, they can be expected to add about eighty per cent at high velocities and somewhat more at low velocities.

An ion carrying a core of more than one electron has states for electron capture all of which are usually very degenerate; moreover, neighboring energy levels are not greatly distant. For these reasons, capture into any particular state is relatively unimportant. Even at high velocities, the principal

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<sup>3</sup> H. C. Brinkman and H. A. Kramers, Proc. K. Akad. Amst. 33, 973 (1930).  
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contributions to the cross section come from excited states.

Since an electron is most readily captured when its velocity is approximately the ion velocity, the momentum distribution of the electrons of the atom from which capture takes place is very important in the capture process. Thus, inner electrons contribute the most to the cross section at high ion velocities and outer electrons the most at low velocities.

In this paper the Born approximation is used to study the capture cross section of high-velocity ions. Because the masses of the ion and atom are very large compared to the electron mass, the atom is considered as stationary and the velocity of the ion regarded as unchanged in the collision process. The transition probability is calculated by the method of impact parameters without requiring conservation of energy<sup>4</sup>. A momentum represen-

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<sup>4</sup> Compare reference 3.

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tation is used for the electrons, which simplifies the calculations and makes possible a simple Thomas-Fermi treatment of the atomic electrons.

## 2. FIRST BORN APPROXIMATION

The capture cross section is

$$\sigma_c = \sum_{\text{states}} \int d\vec{b} |c|^2 \quad (2)$$

where  $\vec{b}$  is the impact parameter ( $\vec{b} \cdot \vec{v} = 0$ ;  $\vec{v}$  is the ion velocity), and  $c$  is the probability amplitude of a final state corresponding to capture. In the initial state the ion is approaching the neutral atom. Its Coulomb field (energy terms  $-ie^2/R$  in the Hamiltonian for each atomic electron, where  $ie$  is the net, or effective, charge of the ion and  $R$  the distance from the ion to the electron) affects the electrons of the atom. Possible final states in the collision correspond to no change, excitation of the ion, further ionization, excitation of the atom, ionization of the atom without capture, and ionization of the atom with capture by the ion.

In the Born approximation, the deformation of the wave functions during impact is neglected. The wave functions are assumed to be nearly orthogonal and all transition probabilities are assumed to be small.

If a Hartree model is used, it is sufficient to consider the electrons separately and introduce statistical factors where necessary. The probability amplitude then is

$$c = \frac{i}{\hbar} \int_{-\infty}^{\infty} dt \int d\vec{r} \psi_a^*(\vec{r}) e^{\frac{i}{\hbar}(\vec{m}\vec{v} \cdot \vec{r})} \frac{1}{R} e^{\frac{i}{\hbar}(E_i - E_a + \frac{1}{2}m v^2)t} \psi_a(\vec{r}) \quad (3)$$

In this formula  $\psi_a(\vec{r})$  and  $\psi_i(\vec{r})$  are solutions of the Schrodinger equation for the electron when bound with energies  $E_a$  and  $E_i$  to the atom and ion, respectively.

A transformation to a momentum representation is convenient because  $R$  contains the time. The following two functions are introduced:

$$\begin{aligned}\phi_a(\vec{p}) &= \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int d\vec{r} \psi_a(\vec{r}) e^{-\frac{i}{\hbar}(\vec{p}\cdot\vec{r})}, \\ \Phi_i(\vec{p}) &= \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int d\vec{R} \frac{e^{i\vec{p}\cdot\vec{R}}}{R} \psi_i(\vec{R}) e^{-\frac{i}{\hbar}(\vec{p}\cdot\vec{R})}\end{aligned}\quad (4)$$

Using  $\vec{R} = \vec{r} + \vec{b} - \vec{v}t$ , the expression for the probability amplitude becomes

$$c = \frac{2\pi i}{V} \int d\vec{p} \Phi_i^*(\vec{p} - m\vec{v}) e^{-\frac{i}{\hbar}(\vec{p}\cdot\vec{b})} \phi_a(\vec{p}) \delta(p_{\parallel} - \frac{mV}{2} - \frac{E_a}{V} + \frac{E_i}{V}), \quad (5)$$

where  $\delta$  is the Dirac delta function and  $p_{\parallel}$  is the component of  $\vec{p}$  parallel to  $\vec{v}$ . In this approximation only electrons for which this component is  $\frac{1}{2}mV + \frac{1}{V}(E_a - E_i) \approx \frac{1}{2}mV$  can undergo capture.

On substitution in (1) there results

$$\sigma_c = \frac{(2\pi)^4 \hbar^2}{V} \sum \int d\vec{p} |\Phi_i(\vec{p} - m\vec{v})|^2 |\phi_a(\vec{p})|^2 \delta(p_{\parallel} - \frac{mV}{2} - \frac{E_a}{V} + \frac{E_i}{V}), \quad (6)$$

where the summation is to be carried out over the occupied states of the atom and the unoccupied states of the ion, each with the factors required by the Hartree model. It is to be noted that

$$(\vec{p} - m\vec{v})^2 - 2mE_i = p^2 - 2mE_a, \quad (7)$$

a relation which greatly simplifies the calculations.

It is interesting to examine (6) for low ion velocities. The principal contributions arise from the maxima of the momentum distributions. Since in general these occur near the origin of



the corresponding momentum space, (6) is large for velocities such that  $\frac{1}{2}mv^2 \approx |E_a - E_i|$ . Hence for a specified pair of states, capture as given by (6) is most probable at low velocities if there is no change in energy of binding and is most probable near that orbital velocity which is the larger if the energy of binding of one state is considerably larger than that of the other.

Cross sections as given by (6) are probably too large because of the error introduced in assuming the amplitude of the initial state to be unity during the collision, for a reduced amplitude for the initial state tends to reduce transition probabilities<sup>3</sup>. Distortions of the momentum distributions to be found in diatomic and polyatomic gases, and in liquids and solids, due to interatomic forces are neglected since they are important only at low velocities, for which calculations have limited validity in the first Born approximation.

## 3. CENTRAL FIELDS

In the central field approximation for the atom and the ion,

$$\begin{aligned}\phi_a(\vec{p}) &= P_{ml}(p) Q_{lm}(u) \bar{F}_m(\phi), \\ \bar{\phi}_i(\vec{p}) &= Q_{m'l'}(p) Q_{l'm'}(u') \bar{F}_{m'}(\phi'),\end{aligned}\quad (8)$$

in which the second and third factors are the usual normalized polar and azimuthal wave functions, respectively, and the first factors are related to the normalized radial wave functions

$R_{ml}(r)$  and  $R_{m'l'}(R)$  through the formulas

$$\begin{aligned}P_{ml}(p) &= \frac{(-i)^l 4\pi}{(2\pi\hbar)^{3/2}} \int_0^\infty d\pi \pi^2 R_{ml}(\pi) j_l\left(\frac{p\pi}{\hbar}\right), \\ Q_{m'l'}(p) &= \frac{(-i)^{l'} 4\pi}{(2\pi\hbar)^{3/2}} \int_0^\infty dR R^2 \frac{ie^2}{R} R_{m'l'}(R) j_{l'}\left(\frac{pR}{\hbar}\right), \\ j_l(p) &= \sqrt{\frac{\pi}{2p}} J_{l+1/2}(p).\end{aligned}\quad (9)$$

The first four polar functions are  $Q_{00}(u) = \frac{1}{\sqrt{2}}$ ,  $Q_{10}(u) = \sqrt{\frac{3}{2}} u$ ,

$$Q_{1\pm 1}(u) = \sqrt{\frac{3}{4}} (1-u^2)^{1/2}.$$

The capture cross section as given by (6) then becomes

$$\sigma_c = \frac{(2\pi)^3 \hbar^2}{v^2} \sum_{p_{11}} \int_{p_{11}}^\infty \frac{dp^2}{2} |Q_{m'l'}(p)|^2 |Q_{l'm'}(u')|^2 |P_{ml}(p)|^2 |Q_{lm}(u)|^2, \quad (10)$$

where

$$\begin{aligned}p_{11} &= \frac{mv}{2} + \frac{1}{v}(E_{ml} - E_{m'l'}), & u &= p_{11}/p, \\ p^2 - 2mE_{m'l'} &= p^2 - 2mE_{ml}, & u' &= (p_{11} - mv)/p,\end{aligned}\quad (11)$$

and the summation is over nlm of the atom and n'l'm' of the ion with appropriate factors.

## 4. PARTICULAR STATES WITH HYDROGEN-LIKE REPRESENTATIONS

The momentum functions of (9) are easily calculated for hydrogen-like states by using the generating functions for the associated Laguerre functions and for the Gegenbauer functions  $C_\mu^\nu(x)$ . The results<sup>5</sup> are

<sup>5</sup> Compare B. Podolsky and L. Pauling, Phys. Rev. 34, 109 (1929).

$$\begin{aligned} P_{nl}(p) &= \frac{(-i)^l \pi l! 2^{2l+1}}{(2\pi\alpha\hbar)^{3/2}} \left[ \frac{n(n-l-1)!}{(n+l)!} \right]^{1/2} \frac{B^l}{(B^2+1)^{l+2}} C_{n-l-1}^{l+1} \left( \frac{B^2-1}{B^2+1} \right), \\ Q_{n'l'}(p) &= ie^2 \alpha' \frac{(-i)^{l'} \pi l'! 2^{2l'+3}}{(2\pi\alpha'\hbar)^{3/2}} \left[ \frac{n'(n'-l'-1)!}{n'(n'+l')!} \right]^{1/2} \frac{B'^{l'}}{(B'^2+1)^{l'+1}} C_{n'-l'-1}^{l'+1} \left( \frac{B'^2-1}{B'^2+1} \right) \end{aligned} \quad (12)$$

where  $\alpha = \frac{Ze}{n} \left( \frac{me^2}{\hbar^2} \right)$ ,  $B = p/\alpha\hbar$ ,  $\alpha' = \frac{ie}{n'} \left( \frac{me^2}{\hbar^2} \right)$ ,  $B' = p/\alpha'\hbar$ .

The energies are  $E_n = -(\alpha\hbar)^2/2m$ ,  $E_{n'} = -(\alpha'\hbar)^2/2m$ . The first three Gegenbauer functions are  $C_0^1(x) = 1$ ,  $C_1^1(x) = 2x$ ,  $C_2^2(x) = 1$ .

The capture cross section into a state  $n'l'm'$  of the ion from a state  $nlm$  of the atom is

$$\begin{aligned} \sigma_e(n'l'm', nlm) &= \pi a_0^2 i^2 \frac{2^8 (e^2/\hbar)^4}{v^2 v_n'^2} \left( \frac{v_n'}{v_n} \right)^5 \left[ \frac{n(n'-l'-1)! (n-l-1)! (l'! l!)}{n'(n'+l')! (n+l)!} \right]^2 2^{4l'+4l} \\ &\int_{B_n^2}^{\infty} dB^2 \frac{1}{(1+B^2)^6} \left\{ 2 \left( \frac{B'}{B'^2+1} \right)^l C_{n'-l'-1}^{l'+1} \left( \frac{B'^2-1}{B'^2+1} \right) Q_{l'm'}(\mu') \left( \frac{B}{B^2+1} \right)^l C_{n-l-1}^{l+1} \left( \frac{B^2-1}{B^2+1} \right) Q_{lm}(\mu) \right\}^2. \end{aligned} \quad (13)$$

In this expression  $v_n = \frac{Ze}{n} \left( \frac{e^2}{\hbar} \right)$  and  $v_{n'} = \frac{ie}{n'} \left( \frac{e^2}{\hbar} \right)$  are the root mean square velocities of the electron in its hydrogen-like orbits in the atom and ion, respectively. Other quantities are

$$\ell_{11} = \frac{1}{2} \left[ \frac{V}{V_n} - \frac{V_n}{V} \left( 1 - \frac{V_n^2}{V^2} \right) \right], \quad \mu = \ell_{11} / \ell, \quad (14)$$

$$\ell_{12} = \left( \frac{V_n}{V} \right)^2 (\ell^2 + 1) - 1, \quad \ell'_{11} = \frac{1}{2} \left[ -\frac{V}{V_n} + \frac{V_n}{V} \left( 1 - \frac{V_n^2}{V^2} \right) \right], \quad \mu' = \ell'_{11} / \ell'$$

The equation (13) gives the following expressions for the capture into 1s, 2s, and 2p states of a stripped ion of atomic charge  $Z$  from a 1s state of an atom with effective nuclear charge  $Z_a^*$ :

$$\frac{\sigma_c(100;100)}{\pi a_0^2} = Z^2 \frac{(4e^2/\hbar)^4}{V^2 V_e^2} \frac{1}{5} \left\{ \frac{V_e/V_a}{1 + \frac{1}{4} \left[ \frac{V}{V_a} - \frac{V_a}{V} \left( 1 - \frac{V_e^2}{V_a^2} \right) \right]^2} \right\}^5,$$

$$\frac{\sigma_c(200;100)}{\pi a_0^2} = Z^2 \frac{4(4e^2/\hbar)^4}{V^2 V_e^2} \frac{1}{5} \left\{ \frac{V_e/2V_a}{1 + \frac{1}{4} \left[ \frac{V}{V_a} - \frac{V_a}{V} \left( 1 - \frac{V_e^2}{4V_a^2} \right) \right]^2} \right\}^5.$$

$$\left[ 1 - \frac{5V_e}{3V_a} \left\{ \frac{V_e/2V_a}{1 + \frac{1}{4} \left[ \frac{V}{V_a} - \frac{V_a}{V} \left( 1 - \frac{V_e^2}{4V_a^2} \right) \right]^2} \right\} + \frac{5}{7} \frac{V_e^2}{V_a^2} \left\{ \frac{V_e/2V_a}{1 + \frac{1}{4} \left[ \frac{V}{V_a} - \frac{V_a}{V} \left( 1 - \frac{V_e^2}{4V_a^2} \right) \right]^2} \right\}^2 \right],$$

$$\frac{\sigma_c(210;100)}{\pi a_0^2} = Z^2 \frac{4(4e^2/\hbar)^4}{V^2 V_e^2} \left( \frac{V_e}{2V_a} \right)^5 \frac{1}{7} \frac{\left[ -\frac{2V}{V_e} + \frac{V_e}{2V} \left( 1 - \frac{4V_a^2}{V_e^2} \right) \right]^2}{\left\{ 1 + \frac{1}{4} \left[ \frac{V}{V_a} - \frac{V_a}{V} \left( 1 - \frac{V_e^2}{4V_a^2} \right) \right]^2 \right\}^7}, \quad (15)$$

$$\frac{\sigma_c(21\frac{1}{2};100)}{\pi a_0^2} = Z^2 \frac{4(4e^2/\hbar)^4}{V^2 V_e^2} \left( \frac{V_e}{2V_a} \right)^3 \frac{1}{21} \frac{1}{\left\{ 1 + \frac{1}{4} \left[ \frac{V}{V_a} - \frac{V_a}{V} \left( 1 - \frac{V_e^2}{4V_a^2} \right) \right]^2 \right\}^6},$$

where  $V_a = Z_a^* e^2/\hbar$  and  $V_e = Z e^2/\hbar$

The formula given above for capture into a 1s state was first derived by Brinkman and Kramers<sup>3</sup>, replacing a less accurate formula of Oppenheimer<sup>1</sup>. The formulas for capture into 2p states were first derived by Saha and Bazu<sup>6</sup>.

<sup>6</sup> M. N. Saha and D. Bazu, Ind. J. Phys. 19, 121 (1945).

For  $v/2v_e \gg 1$ , the Brinkman-Kramers formula becomes

$$\frac{\sigma_c(100;100)}{\pi a_0^2} = Z^2 \frac{(4e^2/k)^4}{V^2 V_e^2} \frac{1}{5} \left(\frac{2V_e}{V}\right)^5 \left(\frac{2V_e}{V}\right)^5 \quad (16)$$

In this limit,  $\sigma_c(200;100)$  is smaller than  $\sigma_c(100;100)$  by a factor 1/8;  $\sigma_c(210;100)$  differs from the Brinkman-Kramers formula by  $\frac{5}{14} \left(\frac{2V_e}{V_e}\right)^2 \left(\frac{2V_e}{V}\right)^2$ ; and  $\sigma_c(21 \pm 1; 100)$  by  $\frac{5}{168} \left(\frac{2V_e}{V_e}\right)^2 \left(\frac{2V_e}{V}\right)^2$

Experiments with alpha particles in hydrogen<sup>7</sup> lead to the

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<sup>7</sup> J. O. Jacobsen, Nature 117, 858 (1926), Phil. Mag. 10, 410 (1930).  
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conclusion that the mean free path at NTP is greater than 20 cm at a velocity of  $17.5 \cdot 10^8$  cm/sec. Since there are  $5.37 \cdot 10^{19}$  atoms/cm<sup>3</sup> at NTP, the capture cross section is less than  $0.93 \cdot 10^{-21}$  cm<sup>2</sup> at this velocity. Thus  $\sigma_c / \pi a_0^2 < 1.1 \cdot 10^{-5}$  for  $v/(e^2/h) = 8$ . The Brinkman-Kramers formula gives  $1.2 \cdot 10^{-5}$  for this ratio, in better agreement with experiment than (16), which gives  $2.4 \cdot 10^{-5}$ . Capture into excited states adds at least twenty per cent to these numbers.

It is to be expected that the equations (15) give some indication of the capture process at low velocities. If  $v_a \neq v_e$ , the Brinkman-Kramers formula has a maximum slightly below  $v = |v_a^2 - v_e^2|^{1/2}$  and tends to zero as  $v^3$ . If  $v_a = v_e$ , it has no maximum and becomes infinite as  $1/v^3$ . By way of illustration, curves using these formulas for alpha particles in atomic hydrogen are shown in Fig. 1. The dashed curves are for capture into particular

two-quantum ( $n' = 2$ ) states. The total cross section for capture into two-quantum states is given by curve  $n' = 2$ . Also plotted are curves for capture into all states having principal quantum numbers 3, 4, etc., calculated from (23) below, and the total cross section for capture into any state of the ion (top curve). Since the energy of the two-quantum states of  $\text{He}^+$  is the same as the energy of the ground state of H, the two-quantum states give the principal contribution to the total cross section, except at very high velocities, where capture into the ground state of  $\text{He}^+$  predominates.

### 5. TOTAL CROSS SECTION FOR CAPTURE INTO HYDROGEN-LIKE STATES

As long as the exclusion principle does not interfere, the sum over  $m'$  in (10) is given by the addition theorem

$$\sum_{m'=-\ell'}^{\ell'} \odot_{\ell'm'}^2(\mu') = \frac{2\ell'+1}{2} \quad (17)$$

If in addition the states of the ion are hydrogen-like, the

sum over  $l'$  is given by the second addition theorem

$$\sum_{\ell'=0}^{n'-1} \frac{(2\ell'+1)2^{4\ell'}(\ell'!)^2(\ell'-n'+1)!}{(n'+\ell')!} \left[ \left( \frac{\xi'}{1+\xi'^2} \right)^{\ell'} C_{n'-\ell'-1}^{\ell'+1} \left( \frac{\xi'^{1/2}}{\xi'^2+1} \right) \right]^2 = n' \quad (18)$$

Therefore, using (12),

$$\sum_{\ell'm'} |Q_{n\ell'}(p)|^2 \odot_{\ell'm'}^2(\mu') = \frac{4i^2 e^4 (d'k)^3}{\pi k^2 [(d'k)^2 + p^2]^2} \quad (19)$$

The total cross section for capture into any state of the ion is, in the central field approximation, the sum of contributions for capture into the unoccupied shells of the ion:

$$\sigma_c = \sum_{n'} \sigma_c(n'). \quad (20)$$

If the shell  $n'$  is completely unoccupied and if a hydrogen-like representation for these states is valid, the use of (19) gives

$$\frac{\sigma_c(n')}{\pi a_0^2} = i^2 \frac{(4e^2/k)^4}{V^2 V_{n'}^2} (m V_{n'})^5 \frac{\pi}{16} \sum \int_{p_{11}^2}^{\infty} dp^2 \frac{|P_{n\ell'}(p)|^2 \odot_{\ell'm}^2(\mu)}{[p^2 - 2m E_{n\ell'}]^2}, \quad (21)$$

where  $V_{n'} = ie^2/n'\hbar$ ,  $p_{11} = \frac{mV}{2} + \frac{1}{V} (E_{n\ell'} + \frac{mV_{n'}^2}{2})$ ,  $\mu = p_{11}/p$ , and the summation is over the  $n\ell m$  states of the atom with appropriate factors.

Since for a 1s state

$$|P_{10}(p)|^2 Q_{00}^2(\mu) = \frac{16}{\pi} \frac{(\alpha \hbar)^5}{[(\alpha \hbar)^2 + p^2]^4}, \quad (22)$$

$$\text{where } \alpha \hbar = m v_a, \quad v_a = Z_a e^2 / \hbar, \quad (21)$$

becomes for an atom with a single 1s electron

$$\frac{\sigma_c(n')}{\pi a_0^2} = i^2 \frac{(4e^2/\hbar)^4}{V^2 V_{n'}^2} \frac{1}{5} \left\{ \frac{V_{n'}/v_a}{1 + \frac{1}{4} \left[ \frac{V}{v_a} - \frac{v_a}{V} \left( 1 - \frac{V_{n'}^2}{v_a^2} \right) \right]^2} \right\}^5 \quad (23)$$

which also follows from the first of equations (14) on replacing  $Z$  by 1 and  $v_0$  by  $v_{n'}$ . For large ion velocities (23) depends on  $n'$  as  $1/n'^5$ . Since  $\sum_{n'} \frac{1}{n'^3} = 1.202$  and since capture is principally from 1s states at high velocities (although other states have this general behavior also), capture into excited states add twenty per cent to the cross section for completely stripped ions of high velocity, as has been observed by Oppenheimer<sup>1</sup>.



## 6. HARTREE TREATMENT OF THE ATOM

For atoms with many electrons it is proposed to use simply

$$P_{ml}(p) = \frac{(-i)^l}{(\alpha \hbar)^{3/2}} \left[ \frac{2^{l+5} (l+1)! l!}{\pi (2l+1)!} \right]^{1/2} \frac{\mathcal{G}^l}{(\mathcal{G}^2 + 1)^{l+2}} \quad (24)$$

as the atomic radial momentum functions. In this expression

$$\alpha = \frac{Z_i^*}{m} \left( \frac{m e^2}{\hbar^2} \right) \quad \text{and} \quad \mathcal{G} = p/\alpha \hbar; \text{ Slater's effective charge }^8$$

is used to calculate  $\alpha$ . Since these functions have the property that  $\int_0^\infty dp p^4 |P_{ml}(p)|^2 = (\alpha \hbar)^2$ , it is consistent to take for the energy Slater's value  $E_{ml} = -(\alpha \hbar)^2/2m$ .

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<sup>8</sup> J. C. Slater, Phys. Rev. 36, 57 (1930). For atomic nitrogen,  $Z_a$  is 6.7 for the K shell and 3.9 for the L shell.  
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The corresponding space functions are

$$R_{ml}(r) = \alpha^{3/2} \left[ \frac{2^{2l+3}}{(2l+2)!} \right]^{1/2} (\alpha r)^l e^{-\alpha r}, \quad (25)$$

which differ from Slater's functions in that they have a hydrogen-like form for small  $r$  rather than for large  $r$  (the normalization affects the magnitude in both cases). The Slater functions give reasonable values for sizes of atoms and ions but not always reasonable values for the average momentum. In the problem at hand the latter is of prime importance.

On combining (24) with (19), there is obtained for the cross section for capture of a particular electron in an atomic state  $nlm$  into any unoccupied shell of the ion with principal quantum number  $n'$

$$\frac{\sigma_c(n'; nlm)}{\pi a_0^2} = \frac{i^2 (4e^2/h)^4}{V V_{n'}^2} \left(\frac{V_{n'}}{V_a}\right)^5 2^4 \frac{(l+1)! l!}{(2l+1)!} \int_{f_{11}}^{\infty} d f \frac{f^2}{(1+f^2)^6} \left(\frac{f}{1+f^2}\right)^{2l} 2 Q_{lm}^2(\mu), \quad (26)$$

$$\text{where } V_{n'} = \frac{ie^2}{n'h}, V_a = Z_a^* \frac{e^2}{h}, f_{11} = \frac{1}{2} \left[ \frac{V}{V_a} - \frac{V_a}{V} \left( 1 - \frac{V_{n'}^2}{V_a^2} \right) \right], \mu = \frac{h_{11}}{h}.$$

The integration is easily carried out for particular values of  $lm$ .

Equation (26) has been used to calculate capture cross sections for alpha particles in nitrogen. Since the ground state of atomic nitrogen is  $1s^2 2s^2 2p^3 4s$ , the three  $2p$  electrons have  $m = -1, 0, +1$ . Hence

$$\sigma_c(n') = 2 \sigma_c(n'; 100) + 2 \sigma_c(n'; 200) + \sigma_c(n'; 210) + 2 \sigma_c(n'; 211) \quad (27)$$

In Fig. 2 are plotted cross sections for capture into the ground state only ( $n' = 1$ ) of  $\text{He}^+$  and the total cross section (top curve). The curves for the  $1s^2$  and  $2s^2$  electrons are essentially the same as curves given by Brinkman and Kramers<sup>3</sup>. However these authors omitted contributions from the  $2p^3$  electrons on the ground that contributions from  $p$  electrons are negligible. Such is not the case for  $v/v_e$  below 5 ( $v_e = 2e^2/h$ ). In fact below about 4.2 the formula for  $2p^3$  electrons contributes more than the formula for the  $2s^2$  electrons, and below about 3.2 it contributes more than the formula for the  $1s^2$  electrons. Contributions of excited states to the various cross sections are given in Table 1. Excited states contribute to the total cross section a maximum of about 60 per cent at slightly below  $v/v_e = 2$ . This maximum comes from the  $2p^3$  electrons. Also shown in Fig. 2 are some

Table 1. Capture cross sections for alpha particles in nitrogen, calculated from a Hartree model.  $v_0 = 4.38 \cdot 10^8$  cm/sec is the root mean square velocity of the electron in the lowest state of singly ionized helium.

		$\sigma_0(1s^2)/\pi a_0^2$			$\sigma_0(2s^2)/\pi a_0^2$		
$v/v_0$	$n' = 1$	$n' > 1$	% addition	total	$n' = 1$	$n' > 1$	% addition total
1	.000304	.000032	11	.00034	8.19	5.35	65 13.5
2	.00579	.00092	16	.0067	.188	.108	57 .30
3	.00669	.00130	19	.0080	.00729	.00276	38 .0101
4	.00304	.00065	22	.0037	.000462	.000149	31 .00061
5	.00100	.00022	22	.00122	.0000442	.0000124	28 .000057
6	.000302	.000062	20	.00036	.0000064	.0000015	24 .0000079
		$\sigma_0(2p^3)/\pi a_0^2$			$\sigma_0/\pi a_0^2$		
$v/v_0$	$n' = 1$	$n' > 1$	% addition	total	$n' = 1$	$n' > 1$	% addn. total
1	14.2	5.5	39	19.7	22.4	10.9	49 34
2	.356	.211	59	.57	.550	.320	58 .87
3	.0107	.0045	43	.0152	.0246	.0086	35 .033
4	.000478	.000162	34	.00064	.00398	.00096	24 .0049
5	.0000379	.0000101	27	.000048	.00109	.00024	22 .00133
6	.0000038	.0000009	25	.0000047	.000312	.000064	21 .00038

points from measurements by Rutherford<sup>9</sup> and Jacobsen<sup>10</sup>. Calculated cross sections are larger by a rather big factor over the entire velocity range, the greatest difference being at low velocities, as expected.

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<sup>9</sup> E. Rutherford, Phil. Mag. 47, 277 (1924); data from alpha particles in mica and in air, which substances seem to have similar characteristics.

<sup>10</sup> J. C. Jacobsen; points shown are for air and are those given by Brinkman and Kramers, loc. cit.  
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# 7. ESTIMATES FOR HEAVY IONS

A simplified expression is obtained from (21) by supposing states of the atom with the same principal quantum number to be degenerate, with  $E_{nl} = -m v_n^2/2$ , replacing the sum of  $|P_{nl}(p)|^2 \otimes \tilde{L}_m(\omega)$  over a complete shell by  $2m^{16} \frac{(m v_n)^5}{\pi [(m v_n)^2 + p^2]^4}$ , and approximating the sum over n with integral  $\int dv_n \frac{Z_a^3}{v_n^2} \frac{e^2}{\hbar}$ . The result is

$$\frac{\sigma_e(n')}{\pi a_0^2} \approx i^2 \frac{(2e^2/\hbar)^7}{v v_n^6} (Z_a^*)^3 \frac{4}{45} \left( \frac{v}{2v_n} - \frac{v_n'}{v} \right)^{-9} I \left( \frac{v}{2v_n} - \frac{v_n'}{2v} \right), \quad (28)$$

where  $(Z_a^*)^3$  is an appropriate average of the cube of the effective nuclear charge and

$$I(y) = 9y \int_0^\infty \frac{dx}{(1+x^2)^5} \quad (29)$$

is an integral which approaches unity for large values of its argument. If Slater's values are used and a simple average taken,  $(Z_a^*)^3_{Av} = 128 = (5.03)^3$  for nitrogen. This factor provides a crude explanation for Jacobsen's observation<sup>10</sup> that the mean free path for capture of alpha particles is more than one hundred times greater in hydrogen than in air.

If in (20) the sum over n' is replaced by  $\int_0^{v_e} dv_n' \frac{i'}{v_n'^2} \frac{e^2}{\hbar}$ ,

there is obtained

$$\frac{\sigma_e}{\pi a_0^2} \approx i^3 (Z_a^*)^3_{Av} \frac{(2e^2/\hbar)^8}{v v_e^7} \frac{1}{45} \left( \frac{v}{2v_e} - \frac{v_e}{2v} \right)^{-9} K \left( \frac{v}{2v_e} - \frac{v_e}{2v} \right)$$

in which

$$K(y) = \frac{9}{4} y^9 \left[ -\frac{1}{2(1+y^2)^{3/2}} + \frac{2}{7} \left[ \frac{2^7}{y + \sqrt{1+y^2}} \right]^2 - \int_0^y \frac{dx}{(1+x^2)^4} \right]$$

is an expression which also approaches unity for large values of its argument.

### 8. STATISTICAL TREATMENT OF THE ATOM

In a Thomas-Fermi treatment of the atom,  $|\phi_a(\vec{p})|^2$  in (6) is replaced by  $N(\vec{p}, E_a) \Delta E_a$ , which is the number of electrons in the energy range  $E_a$  to  $E_a + \Delta E_a$  having momenta in unit range about  $\vec{p}$ , and the sum over the occupied states of the atom is replaced by an integral over the energy of the electrons. This procedure yields

$$\sigma_c = \frac{(2\pi)^4 \hbar^2}{V} \sum \int_{-\infty}^0 dE_a \int d\vec{p} |\phi_i(\vec{p} - m\vec{v})|^2 N(\vec{p}, E_a) \delta(E_a - E_i + \frac{mv^2}{2} - p_{||} V) \quad (32)$$

where the summation is now only over the unoccupied states of the ion.

To calculate  $N(\vec{p}, E_a)$ , let  $\chi(r)$  be the electrostatic potential in the atom. The number of electrons in the range  $dr d\vec{p}$  is  $8\pi n^2 dr d\vec{p} / (2\pi\hbar)^3$ . Since  $E_a = \frac{p^2}{2m} - e\chi(r)$ , these have energies in the range  $dE_a = -e \frac{d\chi}{dr} dr$ . Hence

$$N(\vec{p}, E_a) = 8\pi n^2 \left( -\frac{dr}{dE_a} \right) / (2\pi\hbar)^3 \quad (33)$$

where  $r$  is a function of  $e\chi = \frac{1}{2m} (p^2 - 2mE_a)$

On performing the energy integration

$$\sigma_c = \frac{(2\pi)^4 \hbar^2}{V} \sum \int_{-\infty}^{\frac{1}{2}(\frac{mv^2}{2} - E_i)} d p_{||} \int d\vec{p}_\perp |\phi_i(\vec{p} - m\vec{v})|^2 N(\vec{p}, E_i - \frac{mv^2}{2} + p_{||} V) \quad (34)$$

If (19) is used, the summation of  $|\phi_i(\vec{p} - m\vec{v})|^2$  in (32) over a complete set of unoccupied states with principal quantum number  $n'$  gives

$$\frac{8\pi^2 e^4 (mV_{n'})^3}{(2\pi\hbar)^2 [2me\chi]^2}$$

Therefore for capture into such a group of states,

$$\sigma_c(n') = i^2 \frac{2^5 e^2 (mV_{n'})^3}{V \hbar^2} \int_{-\infty}^{\frac{1}{2}(\frac{mv^2}{2} + \frac{mV_{n'}^2}{2})} d p_{||} \pi \int_0^\infty d p_\perp^2 n^2 \left( -\frac{dr}{dE_a} \right) \frac{1}{[2me\chi]^2} \quad (35)$$

In this expression the second integration is transformed into an integration over  $\chi$ . After the order of integration is interchanged, the integration over  $\beta_n$  is simple. If  $V > V_n$ , the result is

$$\sigma_c(n') = i^2 \frac{2^4 \pi e^4 (m V_n)^3}{V m \hbar^3} \int_0^{x'} d\chi \frac{\chi^2}{[e\chi(n)]^2} \left\{ [2me\chi(n) - (m V_n)^2]^{\frac{1}{2}} - [2me\chi(n') + (m V_n)^2]^{\frac{1}{2}} \right\} \quad (36)$$

$$\text{where } 2me\chi(n') = (m V_n)^2 + \left[ \frac{1}{V} \left( \frac{m V^2}{2} - \frac{m V_n^2}{2} \right) \right]^2,$$

The Fermi charge function  $\phi(\chi)$  is introduced by writing

$$\chi = a\beta'x, \quad e\chi(n) = \frac{Z_a e^2}{a\beta'} \frac{\phi(\beta'x)}{x}, \quad (37)$$

in which  $a = \left( \frac{q\pi^2}{128 Z_a} \right)^{\frac{1}{3}} \frac{\hbar^2}{m e^2}$  is the Fermi length and

$\beta' = \frac{Z_a e^2}{a} / \frac{m V_n^2}{2}$  is an energy parameter.

In terms of these quantities,

$$\frac{\sigma_c(n')}{\pi a_0^2} = i^2 \frac{(2e^2/\hbar)^7}{V V_n^6} Z_a^3 \frac{4}{45} \left( \frac{V}{2V_n} - \frac{V_n}{2V} \right)^{-9} I \left( \frac{V}{2V_n} - \frac{V_n}{2V} \beta' \right) \quad (38)$$

where  $(y > 0)$

$$I(y, \beta') = 45 y^9 \int_0^{x'} d\chi \chi^4 \frac{1}{\phi(\beta'x)} \left\{ \left[ \frac{\phi(\beta'x)}{x} - 1 \right]^{\frac{1}{2}} - \left[ \frac{\phi(\beta'x')}{x} - 1 \right]^{\frac{1}{2}} \right\},$$

$$\text{and } \frac{\phi(\beta'x')}{x'} = 1 + y^2.$$

The formula (35) reduces to (88) on replacing  $\phi(\beta'x)$  by  $(Z_a^* x)^{\frac{1}{3}} / Z_a$ .

Moreover,  $I(y, 0) \equiv I(y)$  and  $I(y, \beta')$  approaches  $I(y)$  for  $y \gg \sqrt{\beta'}$ .

If, as in (30), the sum over  $n'$  is replaced by an integral, there is obtained

$$\frac{\tilde{U}_c}{n a^2} = (i z a)^3 \frac{(z e^2 / \hbar)^8}{V V_0^2} \frac{1}{45} \left( \frac{V}{2 V_0} - \frac{V_0}{2 V} \right) K \left( \frac{V}{2 V_0} - \frac{V_0}{2 V} \beta \right), \quad (40)$$

where  $\beta = \frac{z a e^2}{a} / \frac{m \hbar^2}{2}$  and ( $y > 0$ )

$$K(y, \beta) = 45 y^9 \int_0^{\chi_e} d\chi \frac{\chi^4}{\phi(\beta \chi)^2} \left\{ \frac{1}{3} \left[ \frac{\phi(\beta \chi)}{\chi} \right]^{3/2} - \frac{2}{3} \left[ \frac{\phi(\beta \chi)}{\chi} - 1 \right]^{3/2} - \left[ \frac{\chi}{\phi(\beta \chi)} \right]^{1/2} \left[ \frac{\phi(\beta \chi_0)}{\chi_0} - \frac{1}{8} \right] \right\} \\ + 45 y^9 \int_{\chi_0}^{\chi_e} d\chi \frac{\chi^4}{\phi(\beta \chi)^2} \left\{ \frac{4}{3} \left[ \frac{\phi(\beta \chi)}{\chi} \right]^{3/2} + \frac{2}{3} \left[ \frac{\phi(\beta \chi_0)}{\chi_0} \right]^{3/2} - 2 \left[ \frac{\phi(\beta \chi_0)}{\chi_0} \right]^{1/2} \frac{\phi(\beta \chi)}{\chi} \right\} \quad (41)$$

in which  $\chi_0$  and  $\chi_e$  are defined by

$$\frac{\phi(\beta \chi_0)}{\chi_0} = \left[ \frac{y + \sqrt{1+y^2}}{2} \right]^2, \quad \frac{\phi(\beta \chi_e)}{\chi_e} = 1 + y^2.$$

The quantities  $I(y, \beta')$  and  $K(y, \beta)$  have been tabulated for a few values of the parameters in Table 2.



Table 2. Numerical values of  $I(y, \beta')$  and  $K(y, \beta)$ .

y	v/2v	$I(y, 0)$	$I(y, 5)$	$I(y, 10)$	$I(y, 20)$	$K(y, 0)$	$K(y, 5)$	$K(y, 10)$	$K(y, 20)$
1	1.20	0.058	0.0044	0.0018	0.00066	0.107	0.0076	0.0026	0.00088
2	2.12	0.39	0.077	0.040	0.0175	0.48	0.094	0.046	0.0197
3	3.08	0.65	0.26	0.14	0.068	0.72	0.28	0.15	0.071
4	4.06	0.78	0.49	0.85	0.141	0.81	0.47	0.26	0.14

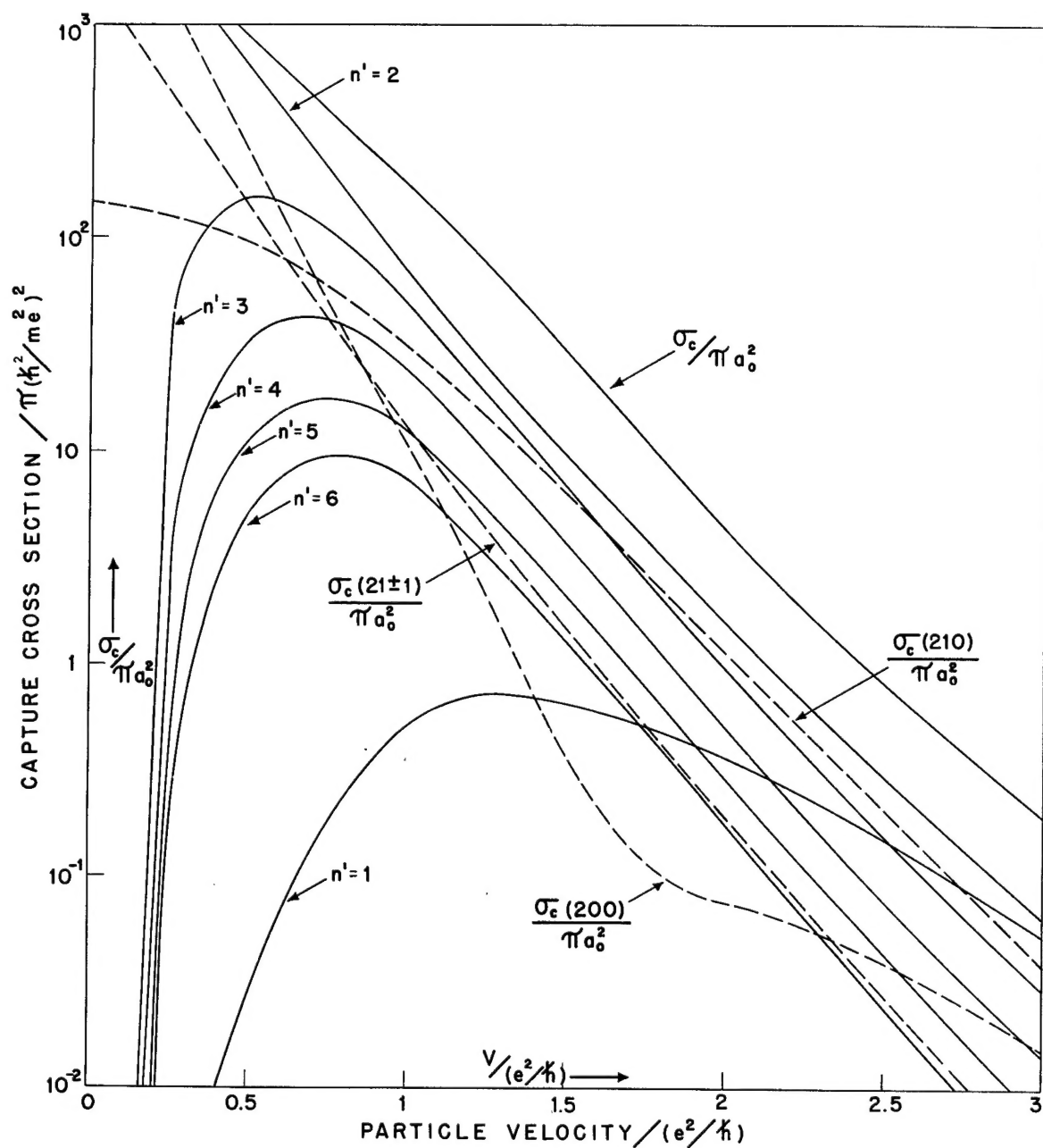


Figure 1.

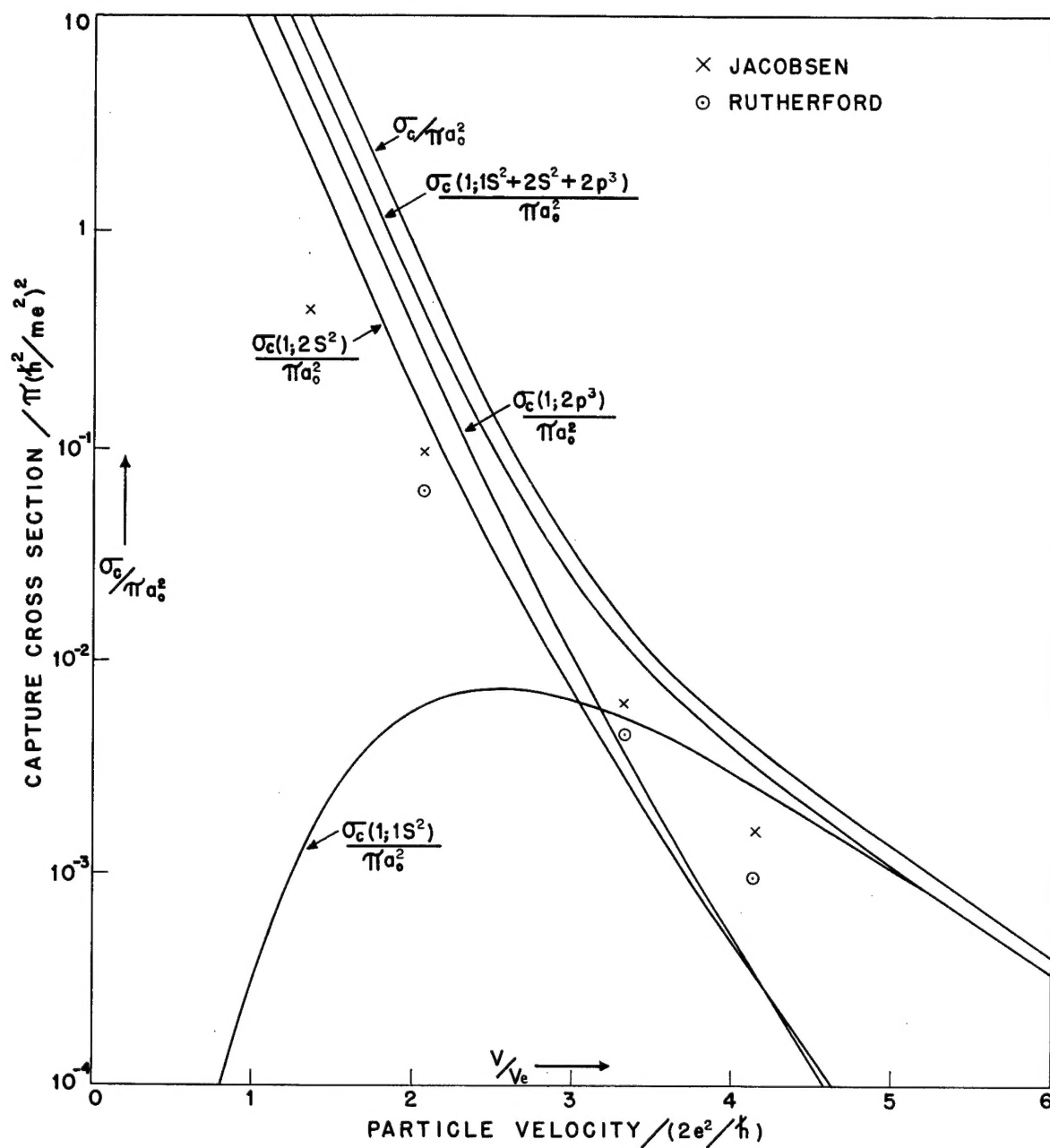


Figure 2.